

Decoherence dynamics of interacting qubits coupled to a bath of local optical phonons

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We study decoherence in an interacting qubit system described by infinite range Heisenberg model (IRHM) in a situation where the system is coupled to a bath of local optical phonons. Using perturbation theory in polaron frame of reference, we derive an effective Hamiltonian that is valid in the regime of strong spin-phonon coupling under non-adiabatic conditions. It is shown that the effective Hamiltonian commutes with the IRHM upto leading orders of perturbation and thus has the same eigenstates as the IRHM. Using a quantum master equation with Markovian approximation of dynamical evolution, we show that the off diagonal elements of the density matrix do not decay in the energy eigen basis of IRHM.

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I. INTRODUCTION

A closed isolated quantum system will always follow unitary quantum dynamics given by Schrodinger equation. However every quantum system that we try to study or model is inevitably coupled to some form of environment and hence an open quantum system [1, 2]. The coupling of a quantum system with its environment leads to decoherence, the process by which information is degraded. Decoherence is the fundamental mechanism by which fragile superpositions are destroyed thereby producing a quantum to classical transition [3, 4]. In fact, decoherence is one of the main obstacles for the preparation, observation, and implementation of multi-qubit entangled states. The intensive work on quantum information and computing in recent years has tremendously increased the interest in exploring and controlling decoherence effects [5–23].

The dynamics of an open quantum system coupled to a bath can be either Markovian or non-Markovian [1, 24–29]. However in this paper we are concerned with the Markovian dynamics of the system infinite range Heisenberg model (IRHM) coupled to a bath of local optical phonons. In case of Markovian processes, the environment acts as a sink for the system information; the system of interest loses information into the environment and this lost information plays no role in the dynamics of the system [1, 30]. Although the theory of decoherence has undergone major advances [3, 4], yet, there exist many definitions of decoherence [31]. For the analysis in this paper, we choose the most commonly used definition of decoherence: Loss of off-diagonal elements in the system's reduced density matrix. In general, a many-qubit

(i.e., many-spin) system can have distance dependent interaction. The two limiting cases for interaction are spin interactions that are independent of distance and spin chains with nearest-neighbor interactions only. In this work we consider the extreme case of distance independent interaction among the spins, i.e., the IRHM.

In this paper, we employ the analytically simpler frame of reference of hard-core-bosons (HCBs) rather than that of spins so that the single particle excitation spectrum can be easily obtained and exploited; we show that the effective Hamiltonian even in higher order (i.e., greater than second order) perturbation theory retains the same eigenstates as the IRHM when the spins are coupled to local phonons. Furthermore, decoherence is studied using the quantum master equation approach [32]. Our analysis based on Markovian quantum master equation shows that the off diagonal matrix elements of density matrix in eigen-basis of IRHM do not decay.

The rest of the paper is organized as follows: In section II, we introduce the IRHM Hamiltonian and map the Hamiltonian to a HCB model. Also in the same section we transform IRHM to a polaron frame using a canonical transformation. In section III, we use second order perturbation theory and with the help of Schrieffer-Wolf (SW) transformation, we derive an effective Hamiltonian that commutes with H_{IRHM} and thus have same set of eigenstates. In section IV, we use the master equation approach and show that the system does not decohere under Markovian approximation. Finally we conclude in section V and make some general remarks regarding the wider context of our results. The paper also contains an Appendix A, where we derive the third order perturbation contribution to our effective Hamiltonian (H_{eff}) and show that the eigenstates of the IRHM Hamiltonian are retained by our H_{eff} .

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II. MODEL HAMILTONIAN FOR THE SYSTEM COUPLED TO A BATH OF PHONONS

We consider a system of spin- $\frac{1}{2}$ particles interacting with each other through a infinite range anisotropic Heisenberg antiferromagnetic exchange interaction i.e. IRHM:

$$H_{\text{IRHM}} = J \sum_{i,j>i} [\vec{S}_i \cdot \vec{S}_j + (\Delta - 1) S_i^z S_j^z] \quad (1)$$

where $J > 0$, $\Delta \geq 0$, and $S_i = \frac{1}{2}\sigma_i$, $i = x, y, z$. We note that H_{IRHM} commutes with both $S_{T\text{total}}^z (\equiv \sum_i S_i^z)$ and $(\sum_i \vec{S}_i)^2 (\equiv S_{T\text{total}}^2)$. In equation (1), it is understood that $J = J^*/(N - 1)$ (where J^* is a finite quantity) so that the energy per site remains finite as $N \rightarrow \infty$. The eigenstates of H_{IRHM} are characterized by S_T (i.e., the total spin eigenvalue) and S_T^z (or the eigenvalue of the z-component of the total spin $S_{T\text{total}}^z$). The ground state corresponds to $S_T^z = 0$ and $S_T = 0$ which is SU(2) invariant.

The IRHM has relevance to many physical problems. The Lipkin-Meshkov-Glick (LMG) model [33] $H_{\text{LMG}} = -2h(\sum_j S_j^z) - 2\lambda[(\sum_j S_j^x)^2 + \gamma(\sum_j S_j^y)^2]/N$ well studied in nuclear many body problem (for $h = 0$ and $\gamma = 1$) is a special case of the above mentioned long-range model for certain set of paramters. It has been shown by Ezawa that the long-range ferromagnetic Heisenberg model describes well a zigzag graphene nanodisc [34]. For spin systems with spins defined on the corners of a regular tetrahedron can be realized (from a Hubbard model) as exact special cases of the above long-range model [35]. In solid state quantum computation using semiconductor quantum dots, spin states are prepared, manipulated, and measured using rapid control of Heisenberg exchange interaction [36].

The real quantum computer will not be free from noise and thus the entangled states have a tendency to undergo decoherence. To study decoherence due to phonons, we consider interaction with optical phonons such as would be encountered when considering transition metal oxides. We write the total Hamiltonian H_T as

$$H_T = H_{\text{IRHM}} + g\omega \sum_i S_i^z (a_i^\dagger + a_i) + \omega \sum_i a_i^\dagger a_i, \quad (2)$$

where a is the phonon destruction operator [37], ω is the optical phonon frequency, and g is the coupling strength. In order to make the calculations simple from spin excitations to particle excitations in our model, we make the mapping of spin operators for spin- $\frac{1}{2}$ particles on HCBs. HCBs are defined on lattice sites $i = 1, \dots, N$ with restricted occupation numbers, $n_i = 0, 1$ [38]. The constrained creation and destruction operators b^\dagger and b , are defined as $b^\dagger = S^+$, $b = S^-$, and $b^\dagger b = S^z + 0.5$. We then observe that conservation of $S_{T\text{total}}^z$ implies conservation of total number of HCB. The total Hamiltonian is then

given by

$$H = J \sum_{i,j>i} [(0.5b_i^\dagger b_j + \text{H.c.}) + \Delta(n_i - 0.5)(n_j - 0.5)] + \omega \sum_j a_j^\dagger a_j + g\omega \sum_j (n_j - \frac{1}{2})(a_j + a_j^\dagger), \quad (3)$$

where $n_j \equiv b_j^\dagger b_j$. Subsequently, we perform the well-known Lang-Firsov (LF) transformation [39, 40] on this Hamiltonian. Under the LF transformation given by $e^S H e^{-S} = H_0 + H_I$ with $S = -g \sum_i (n_i - \frac{1}{2})(a_i - a_i^\dagger)$, the operators b_j and a_j transform like fermions and bosons; this is due to the interesting commutation properties of HCB given below:

$$[b_i, b_j] = [b_i, b_j^\dagger] = 0, \text{ for } i \neq j, \\ \{b_i, b_i^\dagger\} = 1. \quad (4)$$

Next, the unperturbed Hamiltonian H_0 is expressed as [40]

$$H_0 = H_s + H_{\text{env}}, \quad (5)$$

where we identify H_s as the system Hamiltonian

$$H_s = J \sum_{i,j>i} [(0.5e^{-g^2} b_i^\dagger b_j + \text{H.c.}) + \Delta(n_i - 0.5)(n_j - 0.5)], \quad (6)$$

and H_{env} as the Hamiltonian of the environment

$$H_{\text{env}} = \omega \sum_j a_j^\dagger a_j. \quad (7)$$

On the other hand, the interaction H_I which we will treat as perturbation is given by

$$H_I = J \sum_{i,j>i} [0.5e^{-g^2} b_i^\dagger b_j] \{ \mathcal{S}_+^{ij\dagger} \mathcal{S}_-^{ij} - 1 \} + \text{H.c.}, \quad (8)$$

where $\mathcal{S}_\pm^{ij} = \exp[\pm g(a_i - a_j)]$. In the transformed frame, the system Hamiltonian depicts that all the HCBs are coupled to the same phononic mean-field. Thus, the unperturbed Hamiltonian H_0 comprises of the system Hamiltonian H_s representing HCBs with the reduced hopping term $0.5J e^{-g^2}$ and the environment Hamiltonian H_{env} involving displaced bath oscillators corresponding to local distortions. Here it should be pointed out that both the interaction of the HCB with the mean-field as well as the local polaronic distortions in the bath oscillators involve controlled degrees of freedom. Now, the system Hamiltonian H_s can be expressed as

$$H_s = H_{\text{IRHM}} + (H_s - H_{\text{IRHM}}) \quad (9)$$

When we change the Hamiltonian from H_{IRHM} to H_s by adiabatically turning on the perturbation $(H_s - H_{\text{IRHM}})$, the resulting state of the system is still obtainable from

that of H_{IRHM} by using unitary Hamiltonian dynamics and is thus predictable based on a knowledge of the coupling parameter g [41]. Thus no irreversibility is involved in going from H_{IRHM} to H_s . *On the other hand, perturbation H_I pertains to the interaction of HCBs with local deviations from the phononic mean-field; the interaction term H_I represents numerous or uncontrolled environmental degrees of freedom and thus has the potential for producing decoherence.* Furthermore, it is of interest to note that the interaction term is weak in the transformed frame compared to the interaction in the original frame; thus one can perform perturbation theory with the interaction term.

III. EFFECTIVE HAMILTONIAN FROM SECOND ORDER PERTURBATION THEORY

In this section we derive an effective Hamiltonian using second order perturbation theory and Schrieffer-Wolff (SW) transformation. We represent the eigenstates of the unperturbed Hamiltonian H_0 as $|n, m\rangle \equiv |n\rangle_s \otimes |m\rangle_{ph}$ with the corresponding eigenenergies $E_{n,m} = E_n^s + E_m^{ph}$; $|n\rangle_s$ is the eigenstate of the system with eigenenergy E_n^s while $|m\rangle_{ph}$ is the eigenstate for the environment with eigenenergy E_m^{ph} . Henceforth, for brevity, we will use $\omega_m \equiv E_m^{ph}$. On observing that $\langle 0, 0 | H_I | 0, 0 \rangle = 0$ (i.e., the ground state expectation value of the deviations is zero), we obtain the next relevant second-order perturbation term [40]

$$E^{(2)} = \sum_{n,m} \frac{\langle 0, 0 | H_I | n, m \rangle \langle n, m | H_I | 0, 0 \rangle}{E_{0,0} - E_{n,m}}. \quad (10)$$

Employing the SW transformation (see Appendix A of Ref [43]) with the conditions of strong coupling ($g > 1$) and non-adiabaticity ($J^*/\omega \leq 1$), we get the following second-order term $H^{(2)}$ [42]

$$\begin{aligned} H^{(2)} &= - \sum_m \frac{\langle 0 | H_I | m \rangle_{ph} \langle m | H_I | 0 \rangle_{ph}}{\omega_m} \\ &= \sum_{i,j>i} \left[(0.5J_{\perp}^{(2)} b_i^\dagger b_j + \text{H.c.}) \right. \\ &\quad \left. - 0.5J_{\parallel}^{(2)} \{n_i(1-n_j) + n_j(1-n_i)\} \right], \quad (11) \end{aligned}$$

where

$$J_{\perp}^{(2)} \equiv -(N-2)f_1(g) \frac{J^2 e^{-2g^2}}{2\omega} \sim -(N-2) \frac{J^2 e^{-g^2}}{2g^2\omega}, \quad (12)$$

$$J_{\parallel}^{(2)} \equiv [2f_1(g) + f_2(g)] \frac{J^2 e^{-2g^2}}{2\omega} \sim \frac{J^2}{4g^2\omega}, \quad (13)$$

with $f_1(g) \equiv \sum_{n=1}^{\infty} g^{2n}/(n!n)$ and $f_2(g) \equiv \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} g^{2(n+m)}/[n!m!(n+m)]$. The effective Hamiltonian $H_s + H^{(2)}$ is a low energy Hamiltonian

obtained by the canonical SW transformation [44, 45] decoupling the low-energy and the high-energy subspaces; this decoupling is a consequence of $J^* e^{-g^2} \ll \omega$. We now make the important observation that the effective Hamiltonian $H_s + H^{(2)}$, when expressed in terms of spins, has the following form:

$$\sum_{i,j>i} [J_{\text{tr}}(S_i^x S_j^x + S_i^y S_j^y) + J_{\text{lng}} S_i^z S_j^z], \quad (14)$$

and thus has eigenstates identical to those of the original Hamiltonian H_{IRHM} in equation (1) because $\sum_{i,j>i} (S_i^z S_j^z)$ and H_s commute. On carrying out higher order (i.e., beyond second order) perturbation theory (as discussed in Appendix A), and expressing the results in the spin language, we still get an effective Hamiltonian H_{eff} of the following form that has the same eigenstates as the s.

$$\begin{aligned} H_{\text{eff}} &= \sum_{i,j>i} \left[J_{xy} \left(\sum_k S_k^z \right) (S_i^x S_j^x + S_i^y S_j^y) \right] \\ &\quad + \sum_i J_z \left(\sum_k S_k^z \right) S_i^z, \quad (15) \end{aligned}$$

where J_{xy} and J_z are functions of the $S_{\text{Total}}^z (= \sum_k S_k^z)$ operator. It is the infinite range of the Heisenberg model that enables the eigenstates of the system to remain unchanged. Next, we study decoherence in a dynamical context and gain more insight into how the states of our H_s can be decoherence free.

IV. MARKOVIAN DYNAMICS

In this section, we study the markovian dynamics of our system in polaron frame of reference. The dynamics of the system, described by the reduced density matrix $\rho_s(t)$ at time t , is obtained from the density matrix $\rho_T(t)$ of the total system by taking the partial trace over the degrees of freedom of the environment:

$$\rho_s(t) = \text{Tr}_R [\rho_T(t)] = \text{Tr}_R [U(t) \rho_T(0) U^\dagger(t)], \quad (16)$$

where $U(t)$ represents the time-evolution operator of the total system. Now it is evident from the above equation that we need first to determine the dynamics of the total system which is a difficult task in most of the cases. By contrast, master equation approach conveniently and directly yields the time evolution of the reduced density matrix of the system interacting with an environment. This approach relieves us from the need of having to first determine the dynamics of the total system-environment combination and then to trace out the degrees of freedom of the environment.

We consider the following Hamiltonian:

$$H = H_0 + H_I, \quad (17)$$

where H_0 is the system-environment Hamiltonian given by equation (5) and H_I represents the interaction Hamiltonian given by equation (8). Defining an operator O in interaction picture as $\tilde{O} = e^{iH_0 t} O e^{-iH_0 t}$, we write the quantum master equation in Born approximation [1]

$$\begin{aligned} \frac{d\tilde{\rho}_s(t)}{dt} &= -i \text{Tr}_R[\tilde{H}_I(t), \rho_s(0) \otimes R_0] \\ &- \int_0^t d\tau \text{Tr}_R[\tilde{H}_I(t), [\tilde{H}_I(t-\tau), \tilde{\rho}_s(t) \otimes R_0]] \end{aligned} \quad (18)$$

where $R_0 = \sum_n |n\rangle_{ph} \langle n| e^{-\beta\omega_n} / Z$ is the bath density matrix with Z as the partition function. In order to study the Markovian dynamics of the system, we assume that the correlation time scale τ_c for the environmental fluctuations is negligibly small compared to the relaxation time scale τ_s for the system, i.e., $\tau_c \ll \tau_s$. The time scale over

which the system changes is $\tau_s \sim \frac{1}{J^* e^{-g^2}}$ and the bath correlation time scale is $\tau_c \sim \frac{1}{\omega}$. The Markovian approximation is motivated by the condition $J^* e^{-g^2} \ll \omega$ already mentioned in section III. The Markov approximation ($\tau_c \ll \tau_s$) allows us to set the upper limit of the integral to ∞ in equation (18). Thus we obtain the second order time-convolutionless Markovian quantum master equation

$$\begin{aligned} \frac{d\tilde{\rho}_s(t)}{dt} &= -i \text{Tr}_R[\tilde{H}_I(t), \rho_s(0) \otimes R_0] \\ &- \int_0^\infty d\tau \text{Tr}_R[\tilde{H}_I(t), [\tilde{H}_I(t-\tau), \tilde{\rho}_s(t) \otimes R_0]] \end{aligned} \quad (19)$$

Defining $\{|n\rangle_{ph}\}$ as the basis set for phonons, therefore, we can write the master equation as (See Appendix B for details):

$$\begin{aligned} \frac{d\tilde{\rho}_s(t)}{dt} &= - \sum_m \int_0^\infty d\tau [{}_{ph}\langle 0|H_I|m\rangle_{ph}|^2 \tilde{\rho}_s(t) e^{-i\omega_m \tau} + \tilde{\rho}_s(t) {}_{ph}\langle 0|H_I|m\rangle_{ph}|^2 e^{i\omega_m \tau}] \\ &+ \sum_n \int_0^\infty d\tau [{}_{ph}\langle n|H_I|0\rangle_{ph} \tilde{\rho}_s(t) {}_{ph}\langle 0|H_I|n\rangle_{ph} e^{i\omega_n \tau} \\ &\quad + {}_{ph}\langle n|H_I|0\rangle_{ph} \tilde{\rho}_s(t) {}_{ph}\langle 0|H_I|n\rangle_{ph} e^{-i\omega_n \tau}] \\ &= - \sum_n \left[\int_0^\infty d\tau e^{-i(\omega_n - i\eta)\tau} {}_{ph}\langle 0|H_I|n\rangle_{ph}|^2 \tilde{\rho}_s(t) \right. \\ &\quad + \int_0^\infty d\tau e^{i(\omega_n + i\eta)\tau} \tilde{\rho}_s(t) {}_{ph}\langle 0|H_I|n\rangle_{ph}|^2 \\ &\quad \left. - \int_{-\infty}^\infty d\tau e^{i\omega_n \tau} {}_{ph}\langle n|H_I|0\rangle_{ph} \tilde{\rho}_s(t) {}_{ph}\langle 0|H_I|n\rangle_{ph} \right]. \end{aligned} \quad (20)$$

Now, we know $\int_{-\infty}^\infty d\tau e^{i\omega_n \tau} \propto \delta(\omega_n)$. Therefore, on using this relation and the fact that ${}_{ph}\langle 0|H_I|0\rangle_{ph} = 0$, the third term in equation (20) vanishes; hence, we get

$$\frac{d\tilde{\rho}_s(t)}{dt} = i \sum_n \left[\frac{{}_{ph}\langle 0|H_I|n\rangle_{ph}|^2}{\omega_n} \tilde{\rho}_s(t) - \tilde{\rho}_s(t) \frac{{}_{ph}\langle 0|H_I|n\rangle_{ph}|^2}{\omega_n} \right]$$

The term $\sum_n \left[\frac{{}_{ph}\langle 0|H_I|n\rangle_{ph}|^2}{\omega_n} \right]$ corresponds to the effective Hamiltonian $H^{(2)}$ in second order perturbation and commutes with H_0 (see section III). Let $|n\rangle_s$ be the simultaneous eigenstate for $H^{(2)}$ and H_s with eigenvalues $E_n^{(2)}$ and E_n^s , respectively. Then, from the above equation we get:

$${}_s\langle n|\tilde{\rho}_s(t)|m\rangle_s = e^{-i(E_n^{(2)} - E_m^{(2)})t} {}_s\langle n|\tilde{\rho}_s(0)|m\rangle_s, \quad (22)$$

which implies that

$${}_s\langle n|\rho_s(t)|m\rangle_s = e^{-i(E_n - E_m)t} {}_s\langle n|\rho_s(0)|m\rangle_s, \quad (23)$$

where $E_n = E_n^s + E_n^{(2)}$. Thus we see from the above equation that there is only a phase shift but no decoherence! Since the matrix elements of an operator are invariant under canonical transformation, thus under Markovian dynamics, it should be clear that no loss in off-diagonal density matrix elements (i.e., no decoherence) in the LF transformed frame of reference implies no loss in off-diagonal density matrix elements (i.e., no decoherence) in the original untransformed frame of reference. Although the HCB's in the original frame of reference form polarons and are thus entangled with the environment, nevertheless no decoherence results. For greater clarity, we take the example of two qubit state of IRHM i.e. $N=2$. From equation (23), the matrix element ${}_s\langle n|\rho_s(t)|m\rangle_s$ can

be written as

$$\begin{aligned}
{}_s\langle n|\rho_s(t)|m\rangle_s &= {}_s\langle n|\left[\sum_n {}_{ph}\langle n|\rho_T(t)|n\rangle_{ph}\right]|m\rangle_s \\
&= {}_s\langle n|\sum_n {}_{ph}\langle n|e^S\rho_T^o(t)e^{-S}|n\rangle_{ph}|m\rangle_s,
\end{aligned} \tag{24}$$

where $\rho_T^o(t)$ is the total density matrix in the original frame of reference. Now, we illustrate this quantity by considering the simple two-spin (i.e., $N=2$) case of the IRHM. The singlet state $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ and the triplet state $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$ are the $S_T^z = 0$ eigenstates of the two-qubit IRHM Hamiltonian; in HCB language, these states are expressed as $\frac{1}{\sqrt{2}}(|10\rangle - |01\rangle)$ and $\frac{1}{\sqrt{2}}(|10\rangle + |01\rangle)$, respectively. Now, the operator e^{-S} can be expressed as

$$\begin{aligned}
e^{-S} &= e^{g\sum_{i=1,2}(n_i - \frac{1}{2})(a_i - a_i^\dagger)} \\
&= \prod_{i=1,2} e^{g(n_i - \frac{1}{2})(a_i - a_i^\dagger)} \\
&= \prod_{i=1,2} \left[n_i X_i + (1 - n_i) X_i^\dagger \right],
\end{aligned} \tag{25}$$

where $X_i = e^{\frac{g}{2}(a_i - a_i^\dagger)}$. Using the above, we obtain

$$\begin{aligned}
e^{-S} \frac{1}{\sqrt{2}}(|10\rangle \pm |01\rangle)|m_1, m_2\rangle_{ph} \\
= [X_1 X_2^\dagger |10\rangle \pm X_2 X_1^\dagger |01\rangle]|m_1, m_2\rangle_{ph}
\end{aligned} \tag{26}$$

where m_1 and m_2 correspond to phonon occupation numbers at site 1 and site 2 respectively. Therefore, from equation (24) we can write the density matrix element between singlet and triplet states in the original frame of reference as

$$\begin{aligned}
\frac{1}{2} (\langle 10| - \langle 01|) \rho_s(t) (|10\rangle + |01\rangle) \\
= \frac{1}{2} \sum_{m_1, m_2} {}_{ph}\langle m_1, m_2| \left(\langle 10| X_2 X_1^\dagger - \langle 01| X_1 X_2^\dagger \right) \rho_T^o(t) \left(X_1 X_2^\dagger |10\rangle + X_2 X_1^\dagger |01\rangle \right) |m_1, m_2\rangle_{ph}.
\end{aligned} \tag{27}$$

Depending upon the presence or absence of HCB, appropriate deformation will be produced at each site and $\left[\left(X_1 X_2^\dagger |10\rangle \pm X_2 X_1^\dagger |01\rangle \right) |m_1, m_2\rangle_{ph} \right]$ represents polaronic states. Furthermore, in equation (27), no loss in the off-diagonal matrix element on the left hand side implies no loss in the off-diagonal matrix element on the right hand side (i.e., no loss in the measured density matrix elements in the original frame of reference) which in turn means no decoherence results.

Thus, up to second order in perturbation, the assumption $J^* e^{-g^2} \ll \omega$, the infinite range of the Heisenberg model, and the Markov approximation ($\tau_c \ll \tau_s$) together have ensured that the system, with a fixed S_T^z , does not decohere. While the above analysis is valid in the regime $k_B T / \omega \ll 1$, the finite temperature case $k_B T / \omega \gtrsim 1$ needs additional extensive considerations and will be dealt separately.

V. CONCLUSIONS

In conclusion, we have shown that the eigenstates of H_{eff} are the same as those of H_{IRHM} upto the leading order of perturbation. Also we have shown that the off-diagonal elements of the reduced density matrix donot decay in polaron frame of reference, thus no decoherence results. More specifically, for local phonons, ${}_s\langle n|\rho_s(t)|m\rangle_s$ differs from ${}_s\langle n|\rho_s(0)|m\rangle_s$ only by a phase factor and ${}_s\langle n|\rho_s(0)|m\rangle_s$ can be obtained from ${}_s\langle n|\rho_{IRHM}|m\rangle_s$ (density matrix element of IRHM) by an exact unitary evolution [41]. It would be of considerable interest to analyze the non-Markovian decoherence dynamics in the system and is left as future exercise.

Next, our decoherence analysis for local optical phonons will continue to be valid even for the more general optical phonon terms given below:

$$\frac{1}{N^{1/2}} \sum_{i,k} S_i^z [\omega_k (g_k a_{k,i}^\dagger + g_k^* a_{k,i})] + \sum_{k,i} \omega_k a_{k,i}^\dagger a_{k,i}. \tag{28}$$

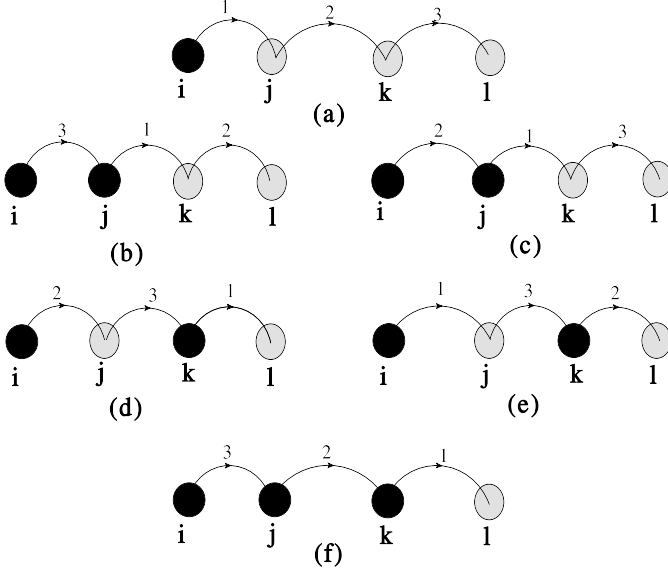


FIG. 1: Open loop hopping processes contributing to effective hopping term T_n^{li} in third-order perturbation theory. Here empty circles correspond to sites with no particles while filled circles correspond to sites with hard-core-bosons. The numbers 1, 2, and 3 indicate the order of hopping.

We also must mention that our approach cannot accommodate the acoustic phonon case as here the condition $J^*e^{-g^2} \ll \omega_k$ cannot be satisfied in the long wavelength limit.

Next, we make a remark on applicability of our model and the decoherence in some real processes. Understanding the highly efficient transport of absorbed light-energy through molecules in photosynthesis is of significant scientific interest and also key to designing light-harvesting technology [46–48]. The model that is used for the study of the excitation energy in Fenna-Matthews-Olson (FMO) complexes is an extreme long range interaction model [48] for excitons with uniform hopping strength between any pair of chromophores in FMO complexes. The phonon fluctuations at various chromophores are uncorrelated to each other [47] i.e., local phonon effects are significant in such complexes. The system-bath coupling in photosynthetic complexes is thought to be not weak but to be at least in the intermediate regime [47]; instead of employing the usual quantum master equation techniques valid for the weak-coupling limit, LF transformed master equation can be used.

Appendix A

In this appendix, we will show that the third-order perturbation theory also produces a term that has the same eigenstates as IRHM. To this end, we obtain the following third-order perturbation term in the effective

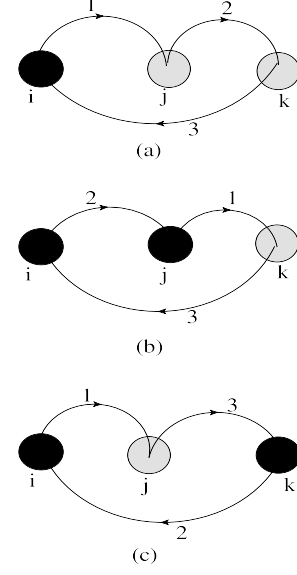


FIG. 2: Closed-loop hopping processes contributing to effective interaction term V_n^i in third-order perturbation theory. Here filled (empty) circles correspond to sites with (without) hard-core-bosons. The numbers 1, 2, and 3 represent hopping sequence.

Hamiltonian:

$$H^{(3)} = \sum_{m \neq 0, n \neq 0} \frac{ph\langle 0|H_I|m\rangle_{ph} \quad ph\langle m|H_I|n\rangle_{ph} \quad ph\langle n|H_I|0\rangle_{ph}}{\Delta E_m^{ph} \Delta E_n^{ph}}. \quad (A1)$$

Here $\Delta E_m^{ph} = \omega_m - \omega_0$. Evaluation of $H^{(3)}$ leads to various hopping terms and interaction terms.

$$H^{(3)} = \sum_{i,l \neq i} \left[\sum_{n=1}^6 t_n T_n^{li} + \sum_{n=1}^3 t_{cn} T_{cn}^{li} \right] + \sum_i \sum_{n=1}^3 v_n V_n^i, \quad (A2)$$

where $t_n \sim (J^3 e^{-g^2})/(g^2 \omega)^2$, $t_{cn} \sim J^3 e^{-g^2}/(g \omega)^2$, and $v_n \sim J^3/(g^2 \omega)^2$ (as will be explained later). We will demonstrate below that $H^{(3)}$ is of the following form

$$H^{(3)} = \sum_{i,l > i} \left[T(\sum_k n_k) b_l^\dagger b_i + \text{H.c.} \right] + \sum_i V(\sum_k n_k) n_i, \quad (A3)$$

where T and V are functions of the total number operator $\sum_k n_k$. Since the IRHM commutes with the total number operator, $H^{(3)}$ has the same eigenstates as IRHM!

There are six open-loop hopping processes T_n^{li} depicted

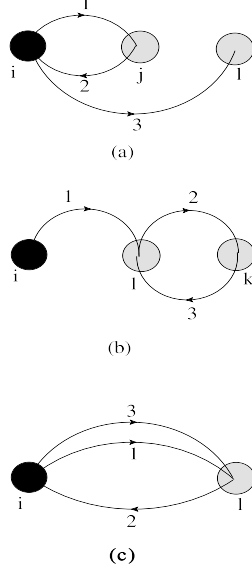


FIG. 3: Hopping processes (involving closed loops) contributing to effective hopping term T_{Cn}^{li} in third-order perturbation theory. Filled (empty) circles represent occupied (unoccupied) sites.

in figure 1. We analyze them sequentially below.

$$\begin{aligned}
 T_1^{li} &= \sum_{k \neq i, l, j} \sum_{j \neq i, l} b_l^\dagger b_k b_k^\dagger b_j b_j^\dagger b_i \\
 &= \sum_{k \neq i, l, j} (1 - b_k^\dagger b_k) \sum_{j \neq i, l} (1 - b_j^\dagger b_j) b_l^\dagger b_i \\
 &= \left[\sum_{k \neq i, l} (1 - b_k^\dagger b_k) - 1 \right] \left[\sum_{j \neq i, l} (1 - b_j^\dagger b_j) \right] b_l^\dagger b_i \\
 &= \left[\sum_{k \neq i, l} (1 - b_k^\dagger b_k) - 1 \right] \left[(N - 2) - \sum_{j \neq l} b_j^\dagger b_j \right] b_l^\dagger b_i \\
 &= \left[\sum_{k \neq i, l} (1 - b_k^\dagger b_k) - 1 \right] \left[(N - 1) - \sum_j b_j^\dagger b_j \right] b_l^\dagger b_i \\
 &= \left[(N - 1) - \sum_j b_j^\dagger b_j \right] \left[\sum_{k \neq i, l} (1 - b_k^\dagger b_k) - 1 \right] b_l^\dagger b_i \\
 &= \left[(N - 1) - \sum_j b_j^\dagger b_j \right] \left[(N - 2) - \sum_k b_k^\dagger b_k \right] b_l^\dagger b_i.
 \end{aligned} \tag{A4}$$

The second hopping process T_2^{li} in figure 1 (b) is given

by

$$\begin{aligned}
 T_2^{li} &= \sum_{k \neq i, l, j} \sum_{j \neq i, l} b_j^\dagger b_i b_l^\dagger b_k b_k^\dagger b_j \\
 &= \sum_{k \neq i, l, j} (1 - b_k^\dagger b_k) \sum_{j \neq i, l} b_j^\dagger b_j b_l^\dagger b_i \\
 &= \sum_{k \neq i, l} (1 - b_k^\dagger b_k) \sum_{j \neq i, l} b_j^\dagger b_j b_l^\dagger b_i \\
 &= \sum_{k \neq i, l} (1 - b_k^\dagger b_k) \left[\sum_j b_j^\dagger b_j - 1 \right] b_l^\dagger b_i \\
 &= \left[\sum_j b_j^\dagger b_j - 1 \right] \left[(N - 1) - \sum_k b_k^\dagger b_k \right] b_l^\dagger b_i. \tag{A5}
 \end{aligned}$$

The hopping process T_3^{li} in figure 1 (c) is expressed as $T_3^{li} = \sum_{k \neq i, l, j} \sum_{j \neq i, l} b_l^\dagger b_k b_j^\dagger b_i b_k^\dagger b_j = T_2^{li}$. The fourth hopping process T_4^{li} in figure 1 (d) is obtained as follows.

$$\begin{aligned}
 T_4^{li} &= \sum_{j \neq i, l, k} \sum_{k \neq i, l} b_k^\dagger b_j b_j^\dagger b_i b_l^\dagger b_k \\
 &= \sum_{j \neq i, l, k} (1 - b_j^\dagger b_j) \sum_{k \neq i, l} b_k^\dagger b_k b_l^\dagger b_i \\
 &= T_2^{li}. \tag{A6}
 \end{aligned}$$

The hopping process T_5^{li} in figure 1 (e) yields $T_5^{li} = \sum_{j \neq i, l, k} \sum_{k \neq i, l} b_k^\dagger b_j b_l^\dagger b_k b_j^\dagger b_i = T_4^{li}$. We analyze below the last hopping process T_6^{li} in figure 1 (f).

$$\begin{aligned}
 T_6^{li} &= \sum_{k \neq i, l, j} \sum_{j \neq i, l} b_j^\dagger b_i b_k^\dagger b_j b_l^\dagger b_k \\
 &= \sum_{k \neq i, l, j} b_k^\dagger b_k \sum_{j \neq i, l} b_j^\dagger b_j b_l^\dagger b_i \\
 &= \left[\sum_{k \neq i, l} b_k^\dagger b_k - 1 \right] \sum_{j \neq i, l} b_j^\dagger b_j b_l^\dagger b_i \\
 &= \left[\sum_{k \neq i, l} b_k^\dagger b_k - 1 \right] \left[\sum_j b_j^\dagger b_j - 1 \right] b_l^\dagger b_i \\
 &= \left[\sum_j b_j^\dagger b_j - 1 \right] \left[\sum_k b_k^\dagger b_k - 2 \right] b_l^\dagger b_i. \tag{A7}
 \end{aligned}$$

We will now deal with closed-loop hopping processes such as those in figure 2. These lead to effective interactions. The process V_1^i in figure 2 (a), obtained from

figure 1 (a) by setting $l = i$, is given as follows.

$$\begin{aligned}
V_1^i &= \sum_{k \neq i, j} \sum_{j \neq i} b_i^\dagger b_k b_k^\dagger b_j b_j^\dagger b_i \\
&= \sum_{k \neq i, j} (1 - b_k^\dagger b_k) \sum_{j \neq i} (1 - b_j^\dagger b_j) b_i^\dagger b_i \\
&= \left[\sum_{k \neq i} (1 - b_k^\dagger b_k) - 1 \right] \left[\sum_{j \neq i} (1 - b_j^\dagger b_j) \right] b_i^\dagger b_i \\
&= \left[(N) - \sum_j b_j^\dagger b_j \right] \left[(N - 1) - \sum_k b_k^\dagger b_k \right] b_i^\dagger b_i \quad (\text{A8})
\end{aligned}$$

Next, the hopping process V_2^i corresponding to closed loop in figure 2 (b) is obtained from figure 1 (c) by taking $l = i$.

$$\begin{aligned}
V_2^i &= \sum_{k \neq i, j} \sum_{j \neq i} b_i^\dagger b_k b_k^\dagger b_j b_j^\dagger b_i \\
&= \sum_{k \neq i, j} (1 - b_k^\dagger b_k) \sum_{j \neq i} b_j^\dagger b_j b_i^\dagger b_i \\
&= \sum_{k \neq i} (1 - b_k^\dagger b_k) \sum_{j \neq i} b_j^\dagger b_j b_i^\dagger b_i \\
&= \sum_{k \neq i} (1 - b_k^\dagger b_k) \left[\sum_j b_j^\dagger b_j - 1 \right] b_i^\dagger b_i \\
&= \left[\sum_j b_j^\dagger b_j - 1 \right] \left[(N) - \sum_k b_k^\dagger b_k \right] b_i^\dagger b_i. \quad (\text{A9})
\end{aligned}$$

Lastly, the hopping V_3^i [depicted by the closed loop in figure 2 (c)] is obtained from figure 1 (e) by setting $l = i$.

$$\begin{aligned}
V_3^i &= \sum_{j \neq i, k} \sum_{k \neq i} b_k^\dagger b_i b_i^\dagger b_k b_j b_j^\dagger b_i \\
&= \sum_{j \neq i, k} (1 - b_j^\dagger b_j) \sum_{k \neq i} b_k^\dagger b_k b_i^\dagger b_i \\
&= V_2^i. \quad (\text{A10})
\end{aligned}$$

Finally, we consider figures 3 (a), (b), and (c) which deal with effective hopping terms T_{Cn}^{li} involving closed loops. The effective hopping term T_{C1}^{li} , corresponding to figure 3 (a), is obtained by setting $k = i$ in figure 1 (a):

$$\begin{aligned}
T_{C1}^{li} &= \sum_{j \neq i, l} b_l^\dagger b_i b_i^\dagger b_j b_j^\dagger b_i \\
&= \sum_{j \neq i, l} (1 - b_j^\dagger b_j) b_l^\dagger b_i \\
&= \left[(N - 2) - \sum_{j \neq l} b_j^\dagger b_j \right] b_l^\dagger b_i \\
&= \left[(N - 1) - \sum_j b_j^\dagger b_j \right] b_l^\dagger b_i. \quad (\text{A11})
\end{aligned}$$

To obtain the effective hopping term T_{C2}^{li} corresponding to figure 3 (b), we take $j = l$ in figure 1 (a):

$$\begin{aligned}
T_{C2}^{li} &= \sum_{k \neq i, l} b_l^\dagger b_k b_k^\dagger b_l b_l^\dagger b_i \\
&= \sum_{k \neq i, l} (1 - b_k^\dagger b_k) b_l^\dagger b_i \\
&= \left[(N - 2) - \sum_{k \neq l} b_k^\dagger b_k \right] b_l^\dagger b_i \\
&= \left[(N - 1) - \sum_k b_k^\dagger b_k \right] b_l^\dagger b_i \\
&= T_{C1}^{li}. \quad (\text{A12})
\end{aligned}$$

The effective hopping term T_{C3}^{li} depicted in figure 3 (c) [upon setting $k = i$ and $j = l$ in figure 1 (a)] is given by

$$T_{C3}^{li} = b_l^\dagger b_i b_i^\dagger b_l b_l^\dagger b_i = b_l^\dagger b_i. \quad (\text{A13})$$

Thus we have shown that $H^{(3)}$ contains effective hopping terms $\sum_{i, l > i} [T(\sum_k n_k) b_l^\dagger b_i + \text{H.c.}]$ and effective interaction terms $(\sum_i V(\sum_k n_k) n_i)$. Since T and V are functions of the total number operator, $H^{(3)}$ and IRHM have the same eigenstates. These arguments can be extended to even higher-order perturbation theory to show that the effective Hamiltonian (after taking all orders of perturbation into account) will give the same eigenstates as IRHM!

We will now explain the expressions for the coefficients t_n , v_n , and t_{cn} in equation (A2), obtained from third-order perturbation theory, using typical schematic diagrams shown in figure 4 [for details of corresponding diagrams and analysis in second order perturbation, see reference [43]]. We consider two distinct time scales associated with hopping processes between two sites: (i) $\sim 1/(Je^{-g^2})$ corresponding to either full distortion at a site to form a small polaronic potential well (of energy $-g^2\omega$) or full relaxation from the small polaronic distortion and (ii) $\sim 1/J$ related to negligible distortion/relaxation at a site. The coefficient t_n corresponds to the typical dominant distortion processes shown schematically in figure 4 (a) with the pertinent typical hopping processes being depicted in figure 1 (a). In figure 4 (a), after the HCB hops away from the initial site, the intermediate states have the same distortion as the initial state. Next, when the HCB hops to its final site there is a distortion at this final site with a concomitant relaxation at the initial site. Hence the contribution to the coefficient t_n becomes $J/(2g^2\omega) \times J/(2g^2\omega) \times Je^{-g^2} \sim J^3 e^{-g^2}/(g^2\omega)^2$. As regards coefficient v_n , it can be deduced based on the typical dominant hopping-cum-distortion processes depicted in figure 4 (b) which typifies the hopping processes in figure 2 (a). In figure 4 (b), when the particle hops to different sites and reaches finally the initial site, there is no change in distortion at any site. Hence v_n can be estimated to be $J/(2g^2\omega) \times J/(2g^2\omega) \times J \sim J^3/(g^2\omega)^2$.

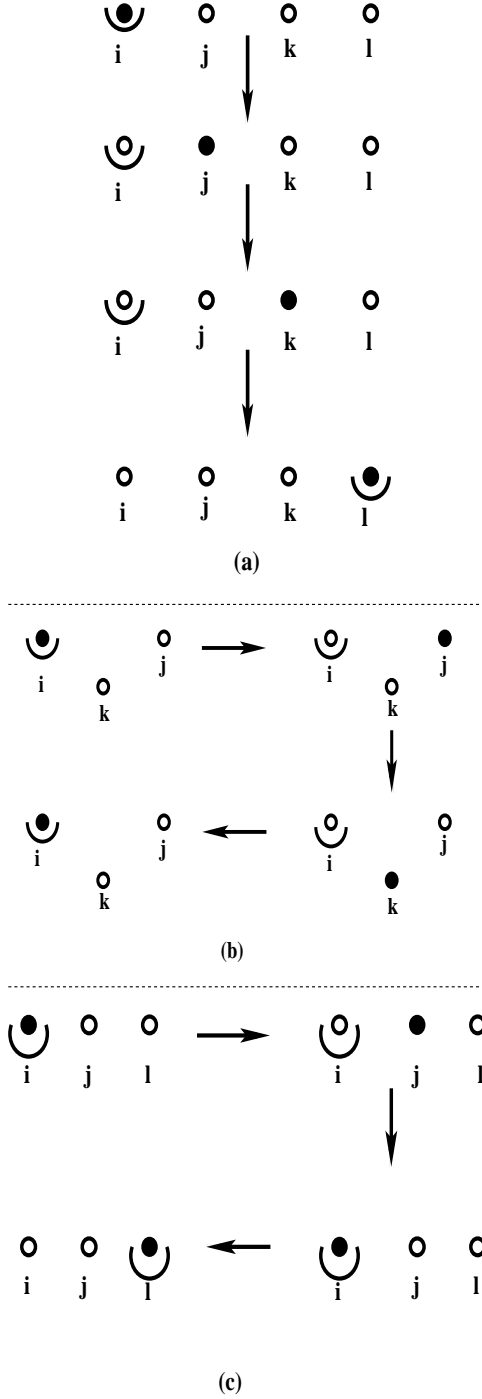


FIG. 4: Schematic diagrams (a), (b), and (c), corresponding to the hopping processes depicted in figure 1 (a), figure 2 (a), and figure 3 (a), respectively, yield coefficients t_n , v_n , and t_{cn} , respectively. The intermediate states give the typical dominant contributions. Here empty circles correspond to empty sites, while filled circles indicate particle positions. Parabolic curve at a site depicts full distortion at that site with corresponding energy $-g^2\omega$ ($+g^2\omega$) if the hard-core-boson is present (absent) at that site.

Lastly, we obtain the coefficient t_{cn} by considering the typical dominant diagram in figure 4 (c) corresponding to the typical process in figure 3 (a). In figure 4 (c), where the first intermediate state depicts the particle hopping but leaving the distortion unchanged, we get a contribution $J/(2g^2\omega)$; for the next intermediate state, where the HCB returns to the initial site, the initial site has to undergo a slight relaxation (involving absorbing a phonon so as to yield a non-zero denominator in the perturbation theory) leading to the contribution J/ω ; and lastly, when the HCB hops to the final site, there is a distortion at the final site with a simultaneous relaxation at the initial site thereby producing a contribution Je^{-g^2} . Thus we calculate t_{cn} to be $J/(2g^2\omega) \times J/\omega \times Je^{-g^2} \sim J^3e^{-g^2}/(g\omega)^2$.

Appendix B

In this appendix we will evaluate the various terms in master equation (19). Defining $\{|n\rangle_{ph}\}$ as the basis set for phonons, therefore, we can write the master equation (equation (19)) as:

$$\begin{aligned}
\frac{d\tilde{\rho}_s(t)}{dt} = & -i \sum_n {}_{ph}\langle n | [\tilde{H}_I(t), \rho_s(0) \otimes R_o] | n \rangle_{ph} \\
& - \sum_n \int_0^\infty d\tau \left[{}_{ph}\langle n | \tilde{H}_I(t) \tilde{H}_I(t-\tau) \tilde{\rho}_s(t) \otimes R_o | n \rangle_{ph} \right. \\
& \quad - {}_{ph}\langle n | \tilde{H}_I(t) \tilde{\rho}_s(t) \otimes R_o \tilde{H}_I(t-\tau) | n \rangle_{ph} \\
& \quad - {}_{ph}\langle n | \tilde{H}_I(t-\tau) \tilde{\rho}_s(t) \otimes R_o \tilde{H}_I(t) | n \rangle_{ph} \\
& \quad \left. + {}_{ph}\langle n | \tilde{\rho}_s(t) \otimes R_o \tilde{H}_I(t-\tau) \tilde{H}_I(t) | n \rangle_{ph} \right]. \tag{B1}
\end{aligned}$$

In order to simplify the above master equation, we need to evaluate the time evolution of the operators involved in H_I . Considering the second term in the equation (B1), yields

$${}_{ph}\langle n | \tilde{H}_I(t) \tilde{H}_I(t-\tau) \tilde{\rho}_s(t) \otimes R_o | n \rangle_{ph} = \sum_m e^{iH_s t} {}_{ph}\langle n | H_I | m \rangle_{ph} e^{-iH_s t} e^{iH_s(t-\tau)} {}_{ph}\langle m | H_I | n \rangle_{ph} e^{-iH_s(t-\tau)} \tilde{\rho}_s(t) \frac{e^{-\beta\omega_n}}{Z} e^{i(\omega_n - \omega_m)\tau}. \tag{B2}$$

In momentum space, we express HCB operators as: $b_j^\dagger = \frac{1}{\sqrt{N}} \sum_k e^{ikr_j} b_k^\dagger$ and $b_j = \frac{1}{\sqrt{N}} \sum_k e^{-ikr_j} b_k$; then, it is important to note that the hopping term in the system Hamiltonian can be written as:

$$\begin{aligned}
0.5J \sum_{i,j>i} (e^{-g^2} b_i^\dagger b_j + \text{H.c.}) &= 0.5J e^{-g^2} \left[\sum_{i,j} b_i^\dagger b_j - \sum_i b_i^\dagger b_i \right] \\
&= 0.5J^* \left(\frac{N}{N-1} \right) e^{-g^2} \hat{n}_0 - 0.5J e^{-g^2} \hat{N}_p \\
&= \sum_k \epsilon_k b_k^\dagger b_k, \tag{B3}
\end{aligned}$$

where we used $J = J^*/(N-1)$, $\hat{N}_p \equiv \sum_k b_k^\dagger b_k$ and $\hat{n}_0 \equiv b_0^\dagger b_0$ (i.e., the particle number in momentum $k=0$ state). Here it should be mentioned that using HCBs instead of spins has enabled us to obtain (with ease) the excitation spectrum ϵ_k which is crucial for the analysis given below. Let $\{|q\rangle_s\}$ denote the complete set of energy eigenstates (with eigenenergies E_q^s) of the system Hamiltonian H_s ; then we can write:

$$\begin{aligned}
e^{iH_s t} H_I e^{-iH_s t} &= 0.5J e^{-g^2} \sum_{l,j>l} \sum_{q,q'} |q\rangle_{ss}\langle q| e^{iH_s t} \left[\frac{1}{N} \sum_{k,p} b_k^\dagger b_p e^{i(kr_l - pr_j)} \right] e^{-iH_s t} |q'\rangle_{ss}\langle q'| \{ \mathcal{S}_+^{lj\dagger} \mathcal{S}_-^{lj} - 1 \} \\
&\quad + \text{H.c.}, \tag{B4}
\end{aligned}$$

which implies

$$e^{iH_s t} {}_{ph}\langle n | H_I | m \rangle_{ph} e^{-iH_s t} = \sum_{q,q'} |q\rangle_{ss}\langle q| {}_{ph}\langle n | H_I | m \rangle_{ph} |q'\rangle_{ss}\langle q'| e^{i(E_q^s - E_{q'}^s)t}, \tag{B5}$$

where $|E_q^s - E_{q'}^s| = 0.5J^* \left(\frac{N}{N-1} \right) e^{-g^2}$ or 0. Here we have taken the total number of HCBs to be conserved; then, only the hopping term in H_s will contribute to the particle excitation energy. Substituting equation (B5) in equation (B2), we get

$$\begin{aligned}
{}_{ph}\langle n | \tilde{H}_I(t) \tilde{H}_I(t-\tau) \tilde{\rho}_s(t) \otimes R_o | n \rangle_{ph} &= \sum_m \sum_{q,q',q''} [\{ |q\rangle_{ss}\langle q| {}_{ph}\langle n | H_I | m \rangle_{ph} |q'\rangle_{ss}\langle q'| {}_{ph}\langle m | H_I | n \rangle_{ph} |q''\rangle_{ss}\langle q''| \} \\
&\quad \times e^{i[(E_q^s - E_{q'}^s)t + (E_{q'}^s - E_{q''}^s)(t-\tau)]} \tilde{\rho}_s(t) \frac{e^{-\beta\omega_n}}{Z} e^{i(\omega_n - \omega_m)\tau} \Big]. \tag{B6}
\end{aligned}$$

Thus under the assumption of $J^*e^{-g^2} \ll \omega$, it follows that $|\omega_n - \omega_m| \gg |E_q^s - E_{q'}^s|$ and $|\omega_n - \omega_m| \gg |E_{q'}^s - E_{q''}^s|$; hence in equation (B6), we can take $e^{i[(E_q^s - E_{q'}^s)t]} = 1$ and $e^{i[(E_{q'}^s - E_{q''}^s)(t-\tau)]} = 1$ which implies that we do not get terms producing decay. The resultant equation is

$${}_{ph}\langle n|\tilde{H}_I(t)\tilde{H}_I(t-\tau)\tilde{\rho}_s(t) \otimes R_o|n\rangle_{ph} = \sum_m {}_{ph}\langle n|H_I|m\rangle_{ph} {}_{ph}\langle m|H_I|n\rangle_{ph} \tilde{\rho}_s(t) \frac{e^{-\beta\omega_n}}{Z} e^{i(\omega_n - \omega_m)\tau}. \quad (\text{B7})$$

Carrying out the same analysis on the remaining (i.e., third, fourth, and fifth) terms in the master equation, we write equation (B1) as:

$$\begin{aligned} \frac{d\tilde{\rho}_s(t)}{dt} = & -i \sum_n {}_{ph}\langle n|[\tilde{H}_I(t), \tilde{\rho}_s(0) \otimes R_o]|n\rangle_{ph} \\ & - \sum_{n,m} \int_0^\infty d\tau \left[{}_{ph}\langle n|H_I|m\rangle_{ph} {}_{ph}\langle m|H_I|n\rangle_{ph} \tilde{\rho}_s(t) \frac{e^{-\beta\omega_n}}{Z} e^{i(\omega_n - \omega_m)\tau} \right. \\ & - {}_{ph}\langle n|H_I|m\rangle_{ph} \tilde{\rho}_s(t) {}_{ph}\langle m|H_I|n\rangle_{ph} \frac{e^{-\beta\omega_m}}{Z} e^{i(\omega_n - \omega_m)\tau} \\ & - {}_{ph}\langle n|H_I|m\rangle_{ph} \tilde{\rho}_s(t) {}_{ph}\langle m|H_I|n\rangle_{ph} \frac{e^{-\beta\omega_m}}{Z} e^{-i(\omega_n - \omega_m)\tau} \\ & \left. + \tilde{\rho}_s(t) {}_{ph}\langle n|H_I|m\rangle_{ph} {}_{ph}\langle m|H_I|n\rangle_{ph} \frac{e^{-\beta\omega_n}}{Z} e^{-i(\omega_n - \omega_m)\tau} \right]. \quad (\text{B8}) \end{aligned}$$

Next, we evaluate the first term in the above equation and show that it is zero at $T = 0$. We observe that

$$\begin{aligned} \text{Tr}_R[\tilde{H}_I(t)R_o] &= \sum_n {}_{ph}\langle n|\tilde{H}_I(t)R_o|n\rangle_{ph} \\ &= 0.5J e^{-g^2} \sum_{l,j \neq l} \left[e^{iH_s t} b_l^\dagger b_j e^{-iH_s t} {}_{ph}\langle 0|\{S_+^{lj\dagger} S_-^{lj} - 1\}|0\rangle_{ph} \right] \\ &= 0. \quad (\text{B9}) \end{aligned}$$

Thus, we have $\sum_n {}_{ph}\langle n|[\tilde{H}_I(t), \rho_s(0) \otimes R_o]|n\rangle_{ph} = 0$ and the master equation at $T = 0$ simplifies as in equation (20).

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